

STN-structure

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L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:331919 CAPLUS

DOCUMENT NUMBER: 143:43819

TITLE: Dipeptidyl peptidase IV inhibitors derived from  $\beta$ -aminoacylpiperidines bearing a fused thiazole, oxazole, isoxazole, or pyrazole

AUTHOR(S): Ashton, Wallace T.; Sisco, Rosemary M.; Dong, Hong; Lyons, Kathryn A.; He, Huaibing; Doss, George A.; Leiting, Barbara; Patel, Reshma A.; Wu, Joseph K.; Marsilio, Frank; Thornberry, Nancy A.; Weber, Ann E.

CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065-0900, USA

SOURCE: Bioorganic &amp; Medicinal Chemistry Letters (2005), 15(9), 2253-2258

CODEN: BMCLE8; ISSN: 0960-894X

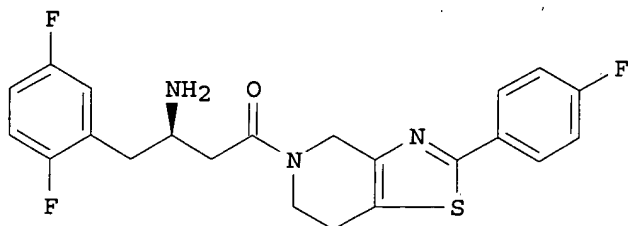
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:43819

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I

AB A series of  $\beta$ -aminoacylpiperidines bearing various fused five-membered heterocyclic rings was synthesized as dipeptidyl peptidase IV inhibitors. Potent and relatively selective inhibition could be obtained, depending on choice of heterocycle, regioisomerism, and substitution. In particular, the analog I (DPP-IV IC<sub>50</sub> = 26 nM) exhibited good oral bioavailability and acceptable half-life in the rat, albeit with rather high clearance.

IT 733758-62-8P 733758-63-9P 733758-64-0P  
733758-65-1P 733758-66-2P 733758-67-3P  
733758-68-4P 733758-69-5P 733758-70-8P  
733758-73-1P 733758-74-2P 733758-75-3P  
733758-76-4P 733758-77-5P 733758-78-6P  
733758-79-7P 733758-80-0P 853784-29-9P  
853784-31-3P 853784-33-5P 853784-37-9P  
853784-38-0P 853784-39-1P 853784-40-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(preparation of dipeptidyl peptidase IV inhibitors derived from  $\beta$ -aminoacylpiperidines bearing a fused thiazole, oxazole, isoxazole, or pyrazole)

RN 733758-62-8 CAPLUS

CN 1H-Pyrazolo[4,3-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-3-methyl- (9CI) (CA INDEX NAME)

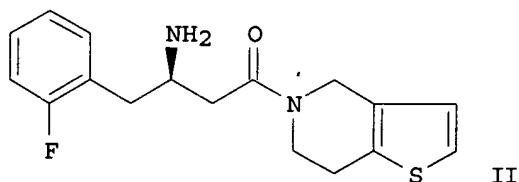
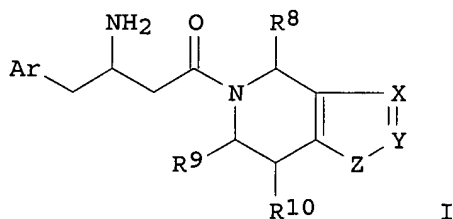
Absolute stereochemistry.

10/542,214

*Interfer*

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2004:633480 CAPLUS  
 DOCUMENT NUMBER: 141:174175  
 TITLE: Preparation of 3-amino-4-phenylbutanoic acid derivatives as dipeptidyl peptidase inhibitors for the treatment or prevention of diabetes  
 INVENTOR(S): Ashton, Wallace T.; Caldwell, Charles G.; Mathvink, Robert J.; Ok, Hyun O.; Reigle, Leah Bitlac; Weber, Ann E.  
 PATENT ASSIGNEE(S): Merck & Co. Inc., USA  
 SOURCE: PCT Int. Appl., 128 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004064778	A2	20040805	WO 2004-US763	20040113
WO 2004064778	A3	20050512		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
AU 2004206812	A1	20040805	AU 2004-206812	20040113
CA 2512546	A1	20040805	CA 2004-2512546	20040113
EP 1589969	A2	20051102	EP 2004-701770	20040113
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006516975	T	20060713	JP 2006-500926	20040113
US 2006069116	A1	20060330	US 2005-542214	20050714
PRIORITY APPLN. INFO.:			US 2003-440732P	P 20030117
			WO 2004-US763	W 20040113
OTHER SOURCE(S):		MARPAT 141:174175		
GI				



AB Title compds. I [X, Y, Z = CR1, NR2, N, O, S, with provisos; Ar = substituted phenyl; R1 = H, halo, OH, CN, alkyl, etc.; R2 = H, alkyl,

alkenyl, etc.; R8-10 = H, CN, alkylcarboxy, etc.] are prepared For instance, a substituted N-Boc protected butanoic acid is coupled to a tetrahydrothieno[3,2-c]pyridine and deprotected to give II. I are inhibitors of the dipeptidyl peptidase-IV enzyme (DP-IV) and which are useful in the treatment or prevention of diseases in which the dipeptidyl peptidase-IV enzyme is involved, such as diabetes and particularly type 2 diabetes.

IT 733758-58-2P 733758-59-3P 733758-60-6P  
 733758-61-7P 733758-62-8P 733758-63-9P  
 733758-64-0P 733758-65-1P 733758-66-2P  
 733758-67-3P 733758-68-4P 733758-69-5P  
 733758-70-8P 733758-73-1P 733758-74-2P  
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 733758-81-1P 733758-82-2P 733758-83-3P  
 733758-84-4P 733758-85-5P 733758-86-6P  
 733758-87-7P 733758-88-8P 733758-89-9P  
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 733758-99-1P

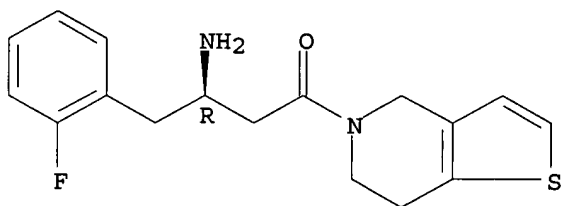
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 3-amino-4-phenylbutanoic acid derivs. as dipeptidyl peptidase inhibitors for treatment or prevention of diabetes)

RN 733758-58-2 CAPLUS

CN Thieno[3,2-c]pyridine, 5-[(3R)-3-amino-4-(2-fluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro- (9CI) (CA INDEX NAME)

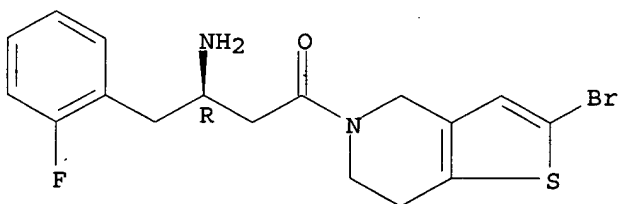
Absolute stereochemistry.



RN 733758-59-3 CAPLUS

CN Thieno[3,2-c]pyridine, 5-[(3R)-3-amino-4-(2-fluorophenyl)-1-oxobutyl]-2-bromo-4,5,6,7-tetrahydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



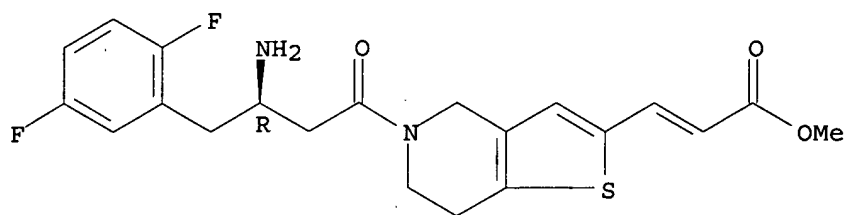
RN 733758-60-6 CAPLUS

CN 2-Propenoic acid, 3-[5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydrothieno[3,2-c]pyridin-2-yl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

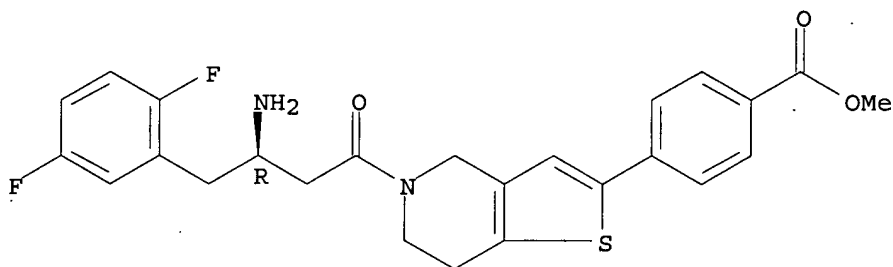
10/542,214



RN 733758-61-7 CAPLUS

CN Benzoic acid, 4-[5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydrothieno[3,2-c]pyridin-2-yl]-, methyl ester (9CI) (CA INDEX NAME)

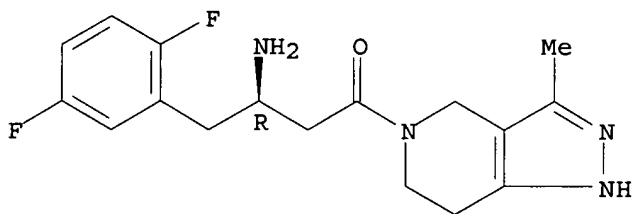
Absolute stereochemistry.



RN 733758-62-8 CAPLUS

CN 1H-Pyrazolo[4,3-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-3-methyl- (9CI) (CA INDEX NAME)

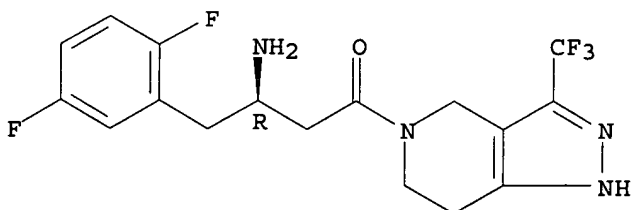
Absolute stereochemistry.



RN 733758-63-9 CAPLUS

CN 1H-Pyrazolo[4,3-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

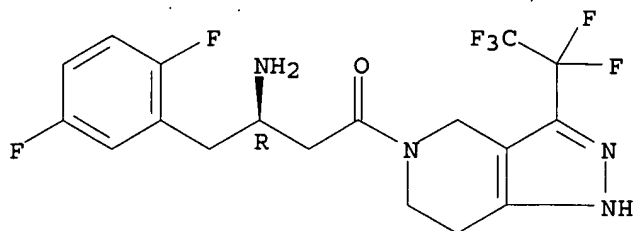


RN 733758-64-0 CAPLUS

10/542,214

CN 1H-Pyrazolo[4,3-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-3-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

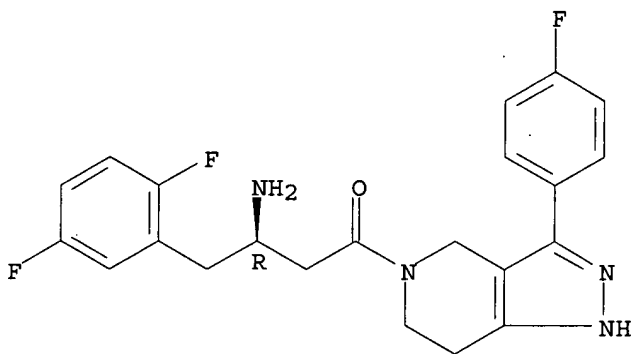
Absolute stereochemistry.



RN 733758-65-1 CAPLUS

CN 1H-Pyrazolo[4,3-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-3-(4-fluorophenyl)-4,5,6,7-tetrahydro- (9CI) (CA INDEX NAME)

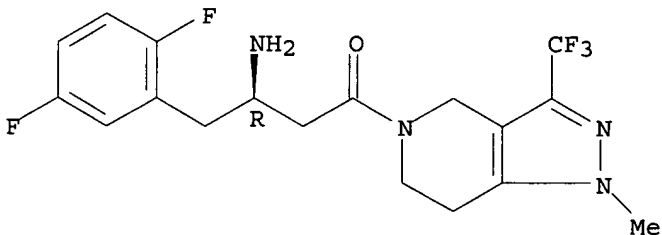
Absolute stereochemistry.



RN 733758-66-2 CAPLUS

CN 1H-Pyrazolo[4,3-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

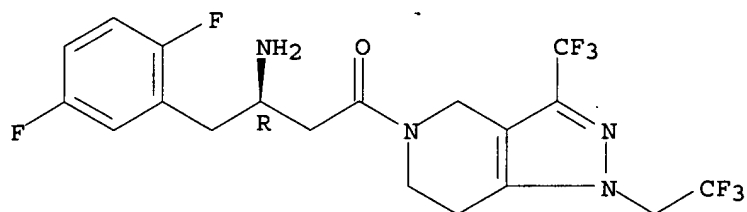


RN 733758-67-3 CAPLUS

CN 1H-Pyrazolo[4,3-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-1-(2,2,2-trifluoroethyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

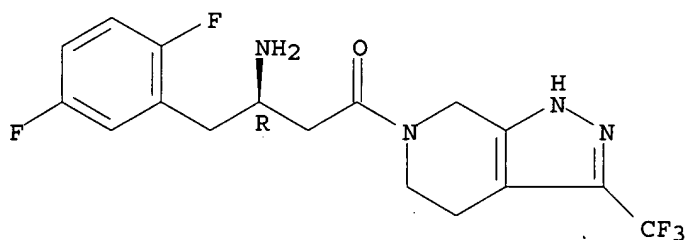
10/542,214



RN 733758-68-4 CAPLUS

CN 1H-Pyrazolo[3,4-c]pyridine, 6-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

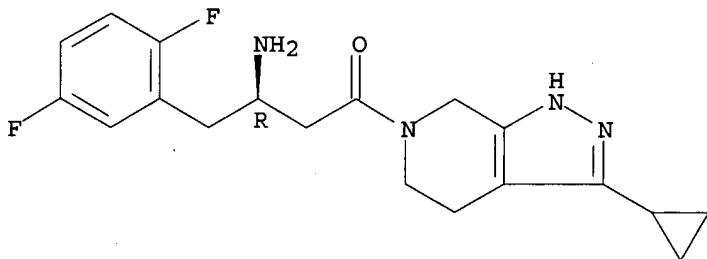
Absolute stereochemistry.



RN 733758-69-5 CAPLUS

CN 1H-Pyrazolo[3,4-c]pyridine, 6-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-3-cyclopropyl-4,5,6,7-tetrahydro- (9CI) (CA INDEX NAME)

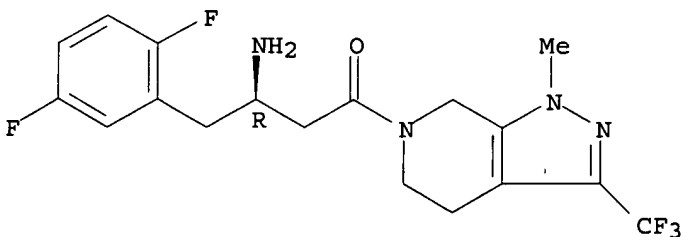
Absolute stereochemistry.



RN 733758-70-8 CAPLUS

CN 1H-Pyrazolo[3,4-c]pyridine, 6-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

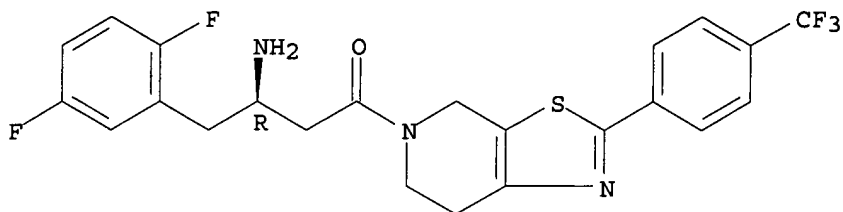


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RN 733758-73-1 CAPLUS

CN Thiazolo[5,4-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-2-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

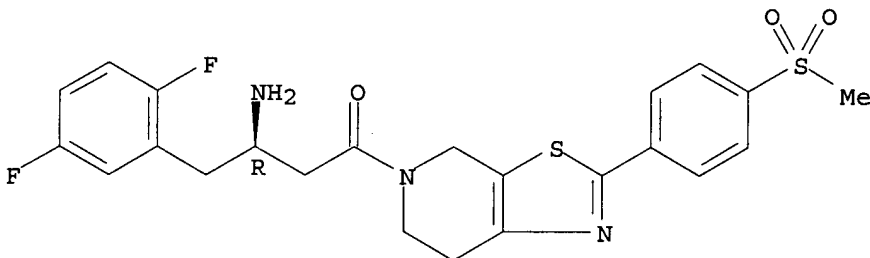
Absolute stereochemistry.



RN 733758-74-2 CAPLUS

CN Thiazolo[5,4-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

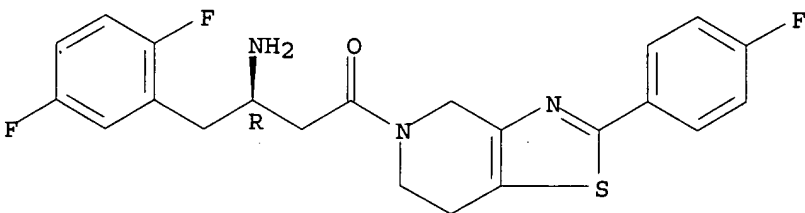
Absolute stereochemistry.



RN 733758-75-3 CAPLUS

CN Thiazolo[4,5-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-2-(4-fluorophenyl)-4,5,6,7-tetrahydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

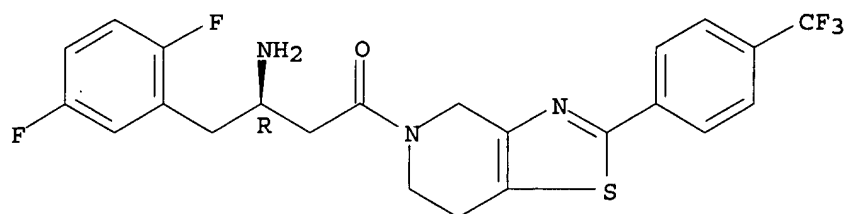


RN 733758-76-4 CAPLUS

CN Thiazolo[4,5-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-2-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

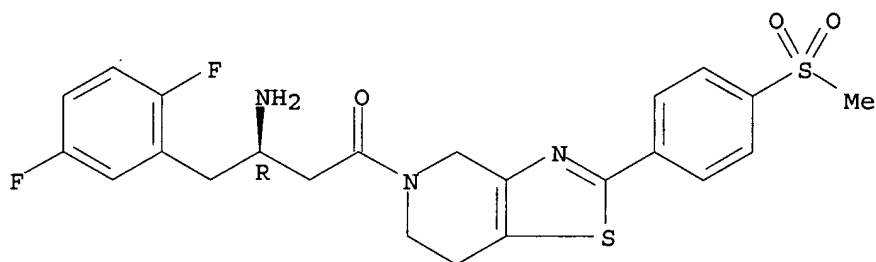
10/542,214



RN 733758-77-5 CAPLUS

CN Thiazolo[4,5-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

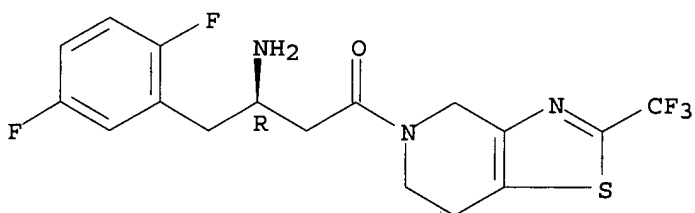
Absolute stereochemistry.



RN 733758-78-6 CAPLUS

CN Thiazolo[4,5-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry..



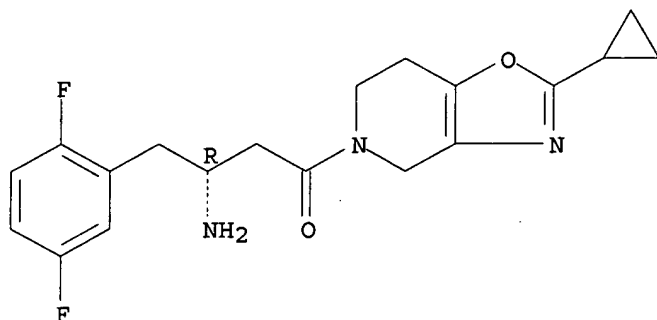
RN 733758-79-7 CAPLUS

CN Oxazolo[4,5-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-2-cyclopropyl-4,5,6,7-tetrahydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



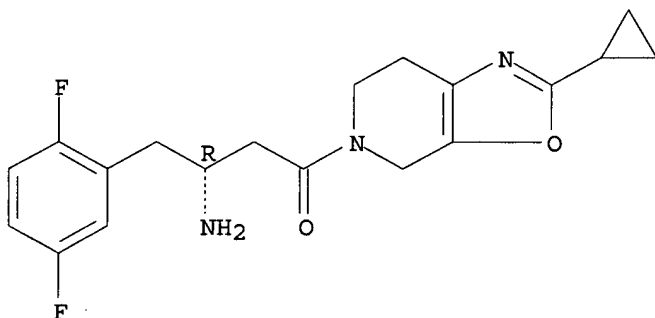
10/542,214



RN 733758-80-0 CAPLUS

CN Oxazolo[5,4-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-2-cyclopropyl-4,5,6,7-tetrahydro- (9CI) (CA INDEX NAME)

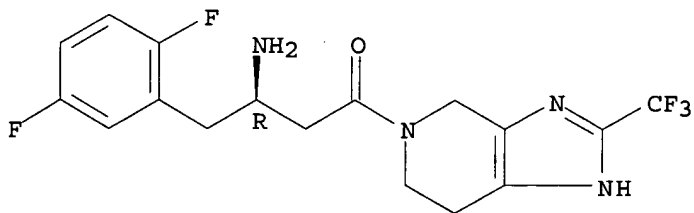
Absolute stereochemistry.



RN 733758-81-1 CAPLUS

CN 1H-Imidazo[4,5-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

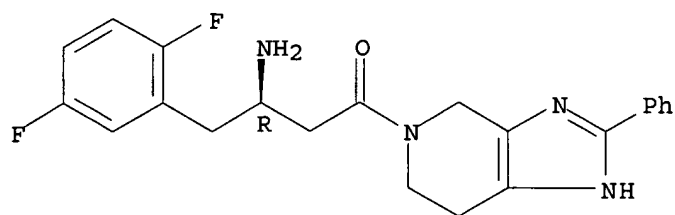


RN 733758-82-2 CAPLUS

CN 1H-Imidazo[4,5-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-2-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

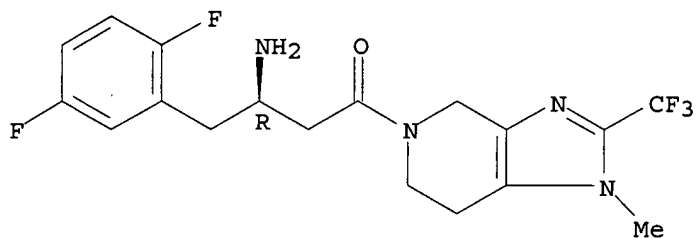
10/542,214



RN 733758-83-3 CAPLUS

CN 1H-Imidazo[4,5-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-1-methyl-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

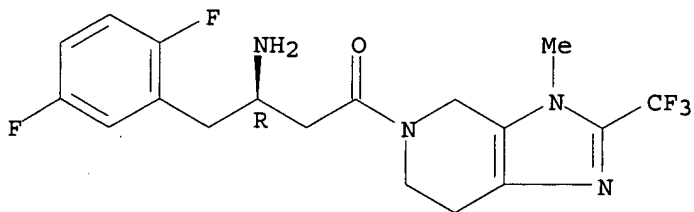
Absolute stereochemistry.



RN 733758-84-4 CAPLUS

CN 3H-Imidazo[4,5-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-3-methyl-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

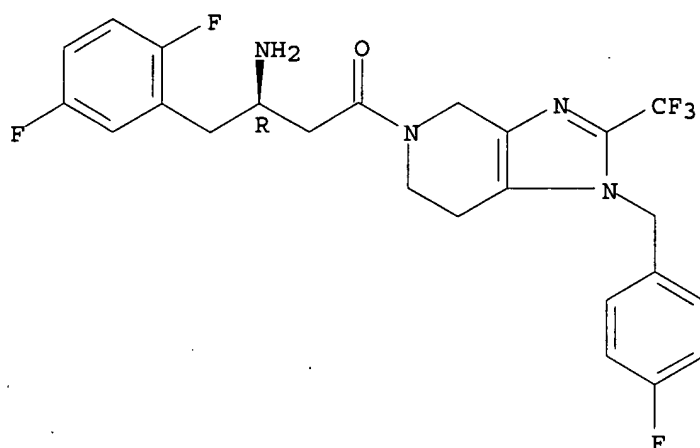


RN 733758-85-5 CAPLUS

CN 1H-Imidazo[4,5-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-1-[(4-fluorophenyl)methyl]-4,5,6,7-tetrahydro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

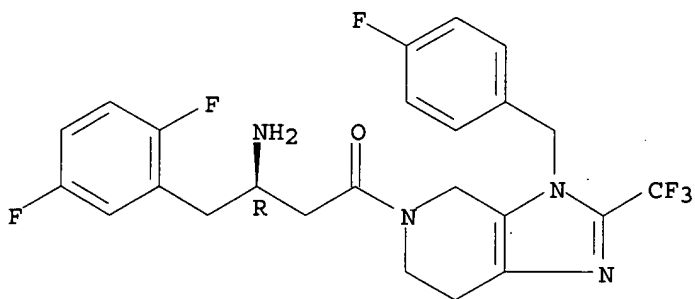
10/542,214



RN 733758-86-6 CAPLUS

CN 3H-Imidazo[4,5-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-3-[(4-fluorophenyl)methyl]-4,5,6,7-tetrahydro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

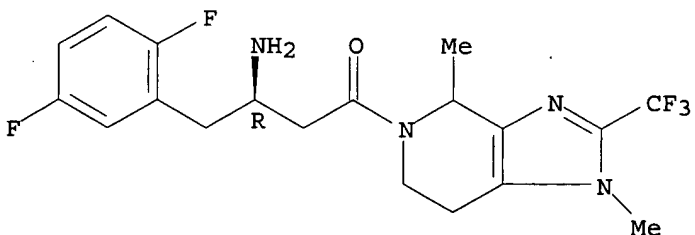
Absolute stereochemistry.



RN 733758-87-7 CAPLUS

CN 1H-Imidazo[4,5-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-1,4-dimethyl-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

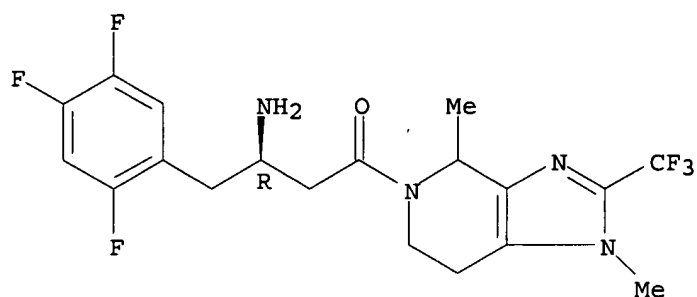


RN 733758-88-8 CAPLUS

CN 1H-Imidazo[4,5-c]pyridine, 5-[(3R)-3-amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-4,5,6,7-tetrahydro-1,4-dimethyl-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

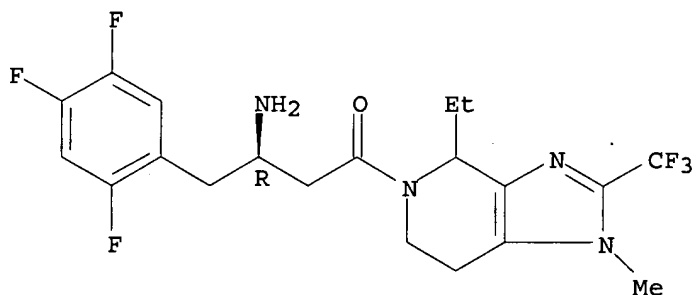
10/542,214



RN 733758-89-9 CAPLUS

CN 1H-Imidazo[4,5-c]pyridine, 5-[(3R)-3-amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-4-ethyl-4,5,6,7-tetrahydro-1-methyl-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

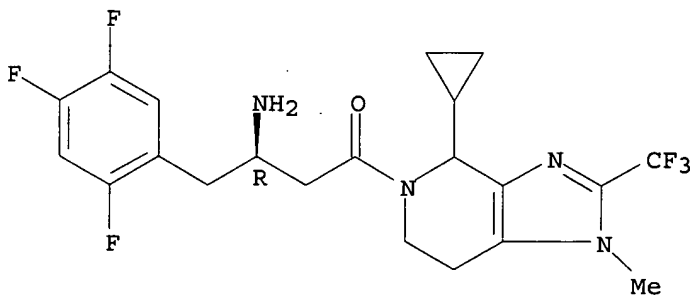
Absolute stereochemistry.



RN 733758-90-2 CAPLUS

CN 1H-Imidazo[4,5-c]pyridine, 5-[(3R)-3-amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-4-cyclopropyl-4,5,6,7-tetrahydro-1-methyl-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

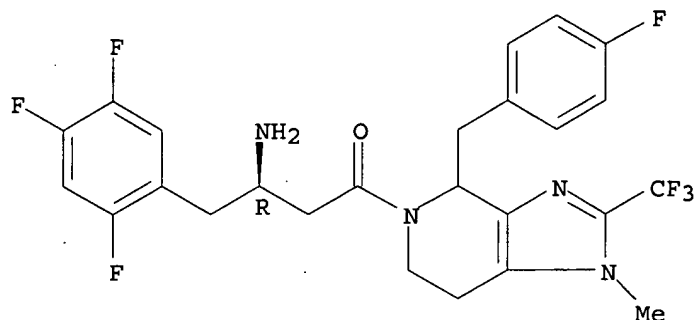


RN 733758-91-3 CAPLUS

CN 1H-Imidazo[4,5-c]pyridine, 5-[(3R)-3-amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-4-[(4-fluorophenyl)methyl]-4,5,6,7-tetrahydro-1-methyl-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

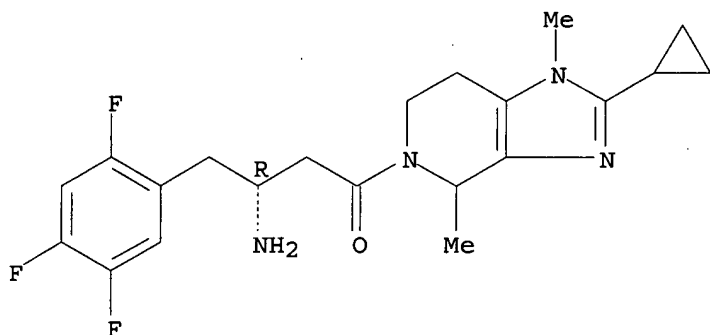
10/542,214



RN 733758-92-4 CAPLUS

CN 1H-Imidazo[4,5-c]pyridine, 5-[(3R)-3-amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-2-cyclopropyl-4,5,6,7-tetrahydro-1,4-dimethyl-(9CI) (CA INDEX NAME)

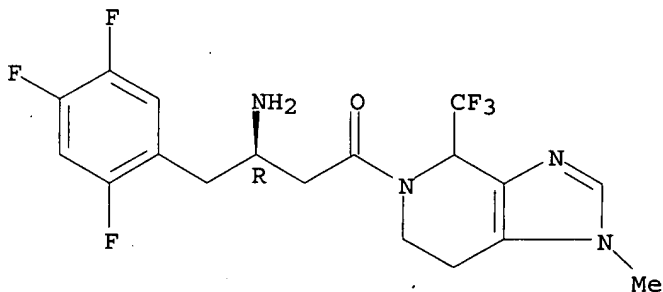
Absolute stereochemistry.



RN 733758-93-5 CAPLUS

CN 1H-Imidazo[4,5-c]pyridine, 5-[(3R)-3-amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-4,5,6,7-tetrahydro-1-methyl-4-(trifluoromethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

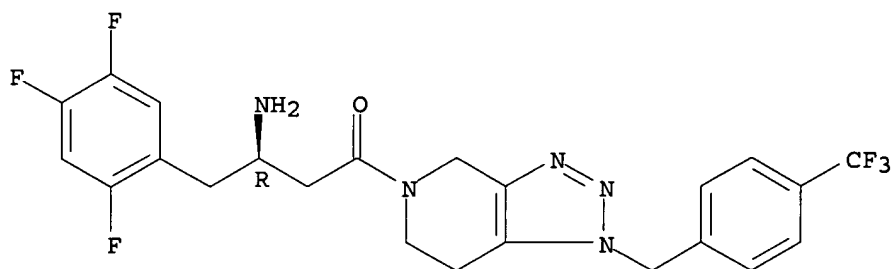


RN 733758-94-6 CAPLUS

CN 1H-1,2,3-Triazolo[4,5-c]pyridine, 5-[(3R)-3-amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-4,5,6,7-tetrahydro-1-[[4-(trifluoromethyl)phenyl]methyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

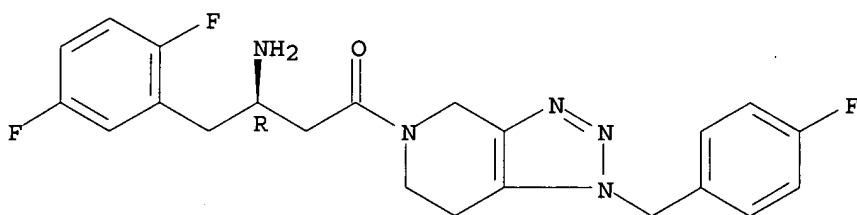
10/542,214



RN 733758-95-7 CAPLUS

CN 1H-1,2,3-Triazolo[4,5-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-1-[(4-fluorophenyl)methyl]-4,5,6,7-tetrahydro- (9CI) (CA INDEX NAME)

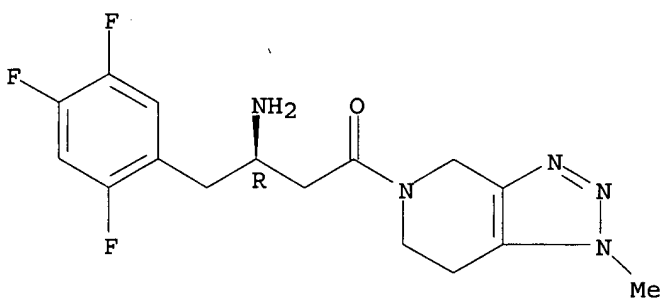
Absolute stereochemistry.



RN 733758-96-8 CAPLUS

CN 1H-1,2,3-Triazolo[4,5-c]pyridine, 5-[(3R)-3-amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-4,5,6,7-tetrahydro-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

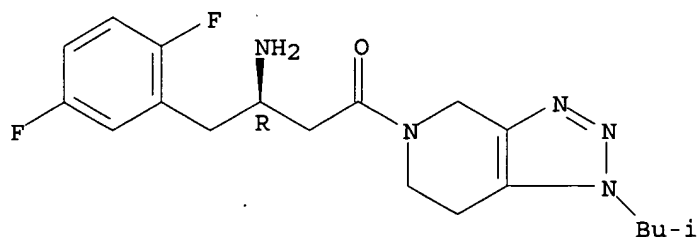


RN 733758-97-9 CAPLUS

CN 1H-1,2,3-Triazolo[4,5-c]pyridine, 5-[(3R)-3-amino-4-(2,5-difluorophenyl)-1-oxobutyl]-4,5,6,7-tetrahydro-1-(2-methylpropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

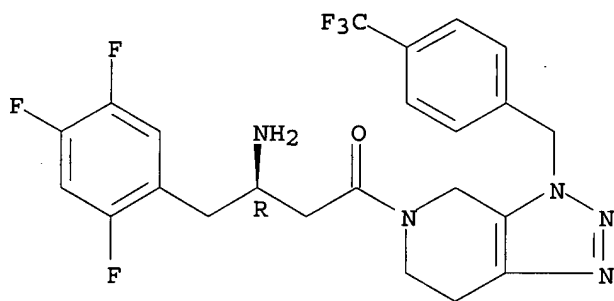
10/542,214



RN 733758-98-0 CAPLUS

CN 3H-1,2,3-Triazolo[4,5-c]pyridine, 5-[(3R)-3-amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-4,5,6,7-tetrahydro-3-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

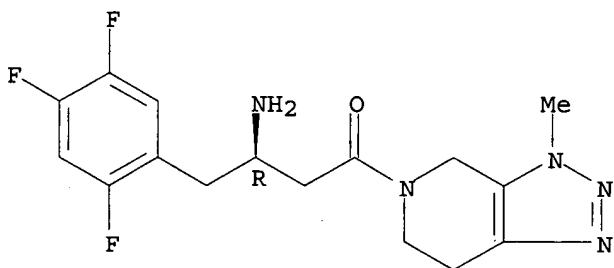
Absolute stereochemistry.



RN 733758-99-1 CAPLUS

CN 3H-1,2,3-Triazolo[4,5-c]pyridine, 5-[(3R)-3-amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-4,5,6,7-tetrahydro-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d his

(FILE 'HOME' ENTERED AT 15:03:31 ON 08 MAR 2007)

FILE 'REGISTRY' ENTERED AT 15:03:45 ON 08 MAR 2007

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 47 S L1 FULL

FILE 'CAPLUS' ENTERED AT 15:04:19 ON 08 MAR 2007

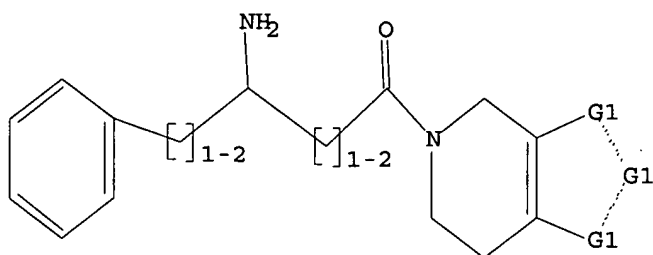
L4 2 S L3

10/542,214

=> d 11

L1 HAS NO ANSWERS

L1 STR



G1 C,O,S,N

Structure attributes must be viewed using STN Express query preparation.

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